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An analytical approach for evaluation of electron capture cross-section using single centre molecular wave function

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Electron capture cross-section in collision of a fast proton with hydrogen molecule using single centered molecular wave function has been done in O.B.K. approximation by Chatterjee *et al* (1971). The above work has been extendes in this paper to obtain a closed form expression for capture cross-section using prior interaction. With single centre wave function which usually have a very large number of terms, an attempt has been made to develop a general expression for cross-section. A summation form for the type integral $G(p, n, k)$, given by Gradshteyn *et al* (1965), has been used. The numerical quadrature for cross-section has been replaced by an analytical method of integration. The final expression for cross-section is directly computable as function of the velocity of incident proton.

1. INTRODUCTION

Electron capture cross-section in collision of a fast proton with hydrogen molecule has been studied by Tuan *et al* (1960), using a two centre molecular wave function for hydrogen molecule. The evaluation of integrals with these wave functions are very tedious and often requires approximation. Another class of wave function defined around a single centre, has been found successful in representing hydrogen molecule and such a wave function has been reported by Bhatia *et al* (1966). Using these single centre wave functions, Chatterjee *et al* (1971), found out cross-section of electron capture at a wide range of high energies of incident proton. The present work is further extension of the above mentioned work, for deriving a closed form analytical expression for cross section. Considering the large ramification in the number of terms of a single centre wave function, the present analytical expression hopes to reduce computation to a substantial amount.

2. Analytical Evaluation of Cross Section

Consider the vector diagram in figure 1. A and B are two protons in the nucleus of the target H_2 molecule, 1 and 2 are its two electrons, C is the incident proton. The capture process may be written as

$$H^+ + H_2 \rightarrow H(1s) + H_2^+$$

If v be the laboratory velocity of the incident proton and μ_i, μ_f the reduced masses in the initial and final systems, the capture cross section may be written as

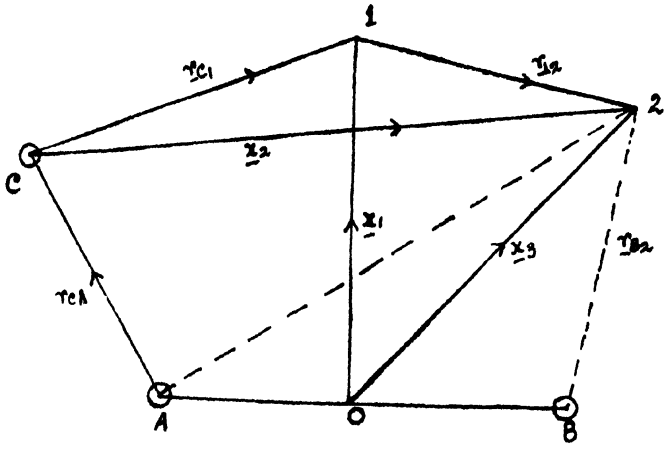
$$Q = \frac{1}{4\pi^2 v^2}\left(\frac{\mu_f}{\mu_i}\right)\int_{p^2_{min}}^{p^2_{max}} |T_i(p^2)|^2 d(p^2)$$

in units of (πa_0^2) (1)

where, $p^2_{min} = (v^2+\epsilon)^2/4v^2$, $p^2_{max} = \infty$, p stands for momentum transfer, ϵ energy discrepancy in Rydbergs and $T_i(p^2)$ the prior transition matrix element.

We shall derive below a closed form expression for capture of electron 2. The single centre wave function for the ground state of hydrogen molecule, is given by

$$\phi_{H_2}(x_1, x_3) = (8\pi^2)^{-\frac{1}{2}} e^{-\gamma(x_1+x_3)} \times \sum_{l,m=0}^{l+m \leqslant w} C_{lm}(x_1^l x_3^m + x_1^m x_3^l) \quad \ldots (2)$$



(Fig 1)

Fig. 1. Vector diagram of colliding system.

The single centre wave function adopted for the ground state of H_2^+ is given by

$$\phi_{H_2^+}(\boldsymbol{x}_1) = (4\pi)^{-\frac{1}{2}}(\alpha_1 e^{-\lambda_1 x_1} + \alpha_2 e^{-\lambda_2 x_1} + \alpha_3 x_1^3 e^{-\lambda_3 x_1}) \quad \ldots (3)$$

where, $\alpha = (9.749, -8.729, -50.5)$, $\lambda = (1.4127, 1.70, 1.00)$

The wave function for Hydrogen atom is

$$\phi_H(\boldsymbol{x}_2) = \frac{1}{\sqrt{\pi}} e^{-x_2} \quad \ldots (4)$$

In the O.B.K. approximation the most important term of prior interaction is $1/x_2$ and with this term we can write down the matrix element $T_i(p^2)$ as

$$T_i(p^2) = \int e^{iz} \phi_{H_2}(\boldsymbol{x}_1 \boldsymbol{x}_3) \phi^*_{H_2^+}(\boldsymbol{x}_1) \phi_H^*(nl, \boldsymbol{x}_2) \frac{1}{x_2} d\boldsymbol{x}_1 d\boldsymbol{x}_2 d\boldsymbol{x}_3 \quad \ldots (5)$$

where, $Z = \boldsymbol{A}_1 \cdot \boldsymbol{x}_1 + \boldsymbol{A}_2 \boldsymbol{x}_2 + \boldsymbol{A}_3 \boldsymbol{x}_3$ and $A_1^2 = 0$, $A_2^2 = p^2$, $A_3^2 = p^2 - \epsilon_{nl}$ and ϵ_{nl} is the energy difference between initial and final state.

The matrix element $T_i(p^2)$ may be expreseed in terms of some basic integrals $G(p, n, \boldsymbol{k})$ as

$$T_i(p^2) = N_1 N_2 N_3 G(1, -1, \boldsymbol{A}_2) \sum_{\substack{l,m \\ m<l}}^{l+m \leq w} C_{lm}[P(l)G(\gamma, m, \boldsymbol{A}_3) + P(m)G(\gamma, l, \boldsymbol{A}_3)] \quad \ldots (6)$$

where, N_1, N_2, N_3 refers to the normalization constants with values

$$N_1 = \frac{1}{\sqrt{\pi}}, \quad N_2 = (8\pi^2)^{-\frac{1}{2}}, \quad N_3 = (4\pi)^{-\frac{1}{2}}$$

$$P(l) = \sum_{i=1}^{3} \alpha_i G(\gamma + \lambda_i, l + n_i, \boldsymbol{A}_1); \qquad n = (0, 0, 3)$$

$$G(p, n, k) = \int e^{i\boldsymbol{k}.\boldsymbol{r}} e^{-pr} r^n dr \quad \ldots (7)$$

$G(p, -1, \boldsymbol{k})$ can be easily evaluated and found to be

$$G(p, -1, \boldsymbol{k}) = \frac{4\pi}{p^2 + k^2} \quad \ldots (8)$$

It is possible to establish a recurrence relation between successive values of $G(p, n, \boldsymbol{k})$ as

$$G(p, n, \boldsymbol{k}) = (-1)^{n+1} \frac{\partial^{n+1}}{\partial p^{n+1}} G(p, -1, \boldsymbol{k}) \quad \ldots (9)$$

Following Gradshteyn *et al* (1965) or by directly computing explicit successive differentiation, it is possible to get,

$$G(\delta_i, l+n_i, \boldsymbol{A}_1) = 4\pi(l+n_i+2)!\,\frac{1}{\delta_i^{l+n_i+3}} \qquad \ldots (10)$$

$$G(\gamma, m, \boldsymbol{A}_3) = \frac{4\pi(m+1)!\gamma^{m+1}}{(\gamma^2+c^2)^{m+2}} \sum_{r=1}^{j} (-1)^{r-1} \binom{m+2}{2r-1} (\gamma^2)^{1-r}(c^2)^{r-1} \qquad \ldots (11)$$

where, $\qquad c^2 = p^2 - \Delta E, \quad j = \mathrm{Int}\left[\frac{m+3}{2}\right]$

writing $C'_{lm} = 2C_{lm}$ if $l = m$ and $C'_{lm} = C_{lm} = C_{ml}$ if $l \neq m$. we have the value of the matrix element given in (6) as,

$$\pi(p^2 = N_1N_2N_3G(1, -1, \boldsymbol{A}_2) \sum_{l=0}^{w} \sum_{m=0}^{w-l} \sum_{i=1}^{3} C'_{lm}\alpha_i G(\delta_i, l+n_i, \boldsymbol{A}_1)G(\gamma, m, \boldsymbol{A}_3)$$

$$= N_1N_2N_3 \frac{64\pi^3}{1+p^2} \sum_{l=0}^{w} \sum_{m=0}^{w-l} C'_{lm} \frac{(m+1)!\gamma^{m+1}}{(\gamma^2+c^2)^{m+2}} \sum_{i=1}^{3} \alpha_i(l+n_i+2)!$$

$$\times \frac{1}{\delta_i^{l+n_i+3}} \sum_{r=1}^{j} (-1)^{r-1} \binom{m+2}{2r-1} (\gamma^2)^{1-r}(p^2-\Delta E)^{r-1} \qquad \ldots (12)$$

The integration of $T_i(p^2)$ over p^2 can be done analytically and may be expressed as,

$$\int |T_i(p^2)|^2 dp^2 = (N_1N_2N_3)^2(64\pi^3)^2 \sum_{l=0}^{w} \sum_{m=0}^{w-l} \sum_{i}^{3} \sum_{r=1}^{j} \sum_{l'=0}^{w} \sum_{m'=0}^{w-l'} \sum_{i'=1}^{3} \sum_{r'=1}^{j'}$$

$$\times \Big[C'_{lm} C''_{l'm'}(m+1)!(m'+1)!\gamma^{m+m'+2}\alpha_i\alpha_{i'}(l+n_i+2)!(l'+n_{i'}+2)!$$

$$\times \frac{1}{\delta_i^{l+n_i+3}\,\delta_{i'}^{l'+n_{i'}+3}} \binom{m+2}{2r-1} \binom{m'+2}{2r'-1} (\gamma)^{4-2(r+r')}$$

$$\times (-1)^{r+r'-2} I_{r+r'-2,\, m+m'+4} \Big] \qquad (13)$$

where,

$$I_{mn} = \int \frac{(x+a)^m dx}{(1+x)^2(x+b)^n} = I_{m-1,\, n-1} - (b-a)I_{m-1,\, n} \qquad \ldots (14)$$

Using the recurrence relation (14), we can find out the value of I_{mn}

$$I_{mn} = \sum_{r=0}^{m} (-1)^r (b-a)^r \binom{m}{r} I_{0,\, n-m+r} \qquad \ldots (15)$$

The integral I_{on} can be further broken into another summation,

$$I_{on} = \frac{n}{n+1} \sum_{L=1}^{n-1} \frac{1}{L(L+1)(b-1)^{n-L}(b+x)^L} + \frac{nI_{01}}{(b-1)^{n-1}} \quad \ldots (16)$$

where,

$$I_{m} = -\frac{1}{(b-1)^2} \log \frac{1+x}{b+x} - \frac{1}{(b-1)(1+x)} \quad \ldots (17)$$

Substituting the limits of integration in equation (13) and multiplying by the constant $\left(\frac{\mu_f}{\mu_i}\right) \cdot \frac{1}{4\pi^2\eta^2}$, we obtain the final expression for cross-section, by using equation (1).

3. Discussion

Although, explicit computation of the value of cross-section for various energies is not yet complete, but the advantage of having analytical expression is quite apparent. Chatterjee and McDowell required numerical differentiations, at the steps (10) and (11). It is well known, that numerical differentiation involves large accumulation of computational error, even in double precision arithmetic in a fast digital computer. The substitution of numerical method by analytical expression is bound to improve accuracy and a lot of saving of computer time. Moreover, the final integral for cross-section given in equation (1) was rdone earlier, by Chatterjee *et al* (1971) by Gaussian Quadratue method. The present paper has reduced the lengthy numerical computation, to the evaluation of expressions given in step (13). Further work along this line hopes to make comparison of the two numerical scheme.

The present method has a large scope of easy generalization to any rearrangement collision of the type,

$$(A+B+e_1+e_2)+C \rightarrow (A+B+e_1)+(C+e_2)$$

In addition to the proposed collision process involving proton and hydrogen molecule, the same expressions with the same single centre molecular wave functions, may be used for the collision between alpha particle and hydrogen molecule. Both the results will be reported shortly after numerical computation. If appropriate single centre wave functions are available then the method can be applied to evaluate capture cross section in ion-atom collisions involving heavy atoms or alkali atoms.

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